

Studies of Mineral Heterogeneity Using the Advanced Light Source

Ardyth M. Simmons¹, William E. Glassley², Geraldine Lamble¹

¹Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

²Earth Sciences Department, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA

Reactive transport simulations have been used in coupling thermohydrologic and chemical (THC) processes to describe the evolution of geothermal fields and potential nuclear waste repositories, ore deposits, and transport at environmentally contaminated sites. Reactive transport models generally use a simplified set of volume-averaged mineral and geochemical parameters as input and then predict the evolution of fluid chemistry and mineralogy along transport pathways. However, naturally heterogeneous distribution of porosity and mineralogy may make volume-averaged representations of those parameters inappropriate, if mineralogy and porosity are correlated. As a result, simulated fluid chemistry may change significantly when represented by volume-averaged vs. non-averaged mineral and porosity distributions. For example, a change in the abundance of ferric minerals can have a noticeable effect on the redox potential of the fluid. As a result of changes in fluid chemistry, mineral dissolution or precipitation can occur. Volumetric mineralogical changes in turn can cause changes to porosity and permeability in the hydrologic framework.

To evaluate this problem, we are working on two dissimilar rock systems. One part of this work addresses the question of the scale of mineralogical heterogeneity that should be included in reactive transport models of THC behavior in fractured volcanic tuffs at Yucca Mountain, Nevada. As a first step, we have determined the compositional heterogeneity of the tuff in order to formulate a means of representing the heterogeneity in a statistical manner (random, fractal, ordered repetition, etc.). We have chosen representative regions of distinct physical properties that represent different types of heterogeneity, including fracture-matrix regions and replacement-alteration regions. The chemical element maps that are produced from probing these regions using the x-ray fluorescence microprobe (beamline 10.3.2) provide a unique means of quantifying the degree of chemical variation across small areas (on the order of less than 1 cm²) that can be compared to larger scale heterogeneities (on the order of 10 m²). Simulations that incorporate small-scale mineralogical differences are then run to determine the sensitivity of model results to these differences. Model output to date suggests the mineralogical results are sensitive to the heterogeneities, implying they must be incorporated in a representative way in larger scale reactive transport simulations in order to obtain realism in modeling the natural system.

A second part of this work addresses the extent to which different fluid chemistries influence the development of mineralogical heterogeneity during recrystallization from the same original bulk composition. We are examining samples of rock which have experienced a uniform temperature and pressure history, but which exhibit different mineralogy. The mineralogy appears to reflect differences in the composition of the co-existing fluid phase from location to location, on the scale of millimeters. By mapping the past distribution of fluid heterogeneity based on differing mineral chemistry, we will be able to establish the scale at which fluid chemistry influences on mineral composition are significant and must be accounted for in reactive transport models.

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Principal investigator: Ardyth Simmons, Earth Sciences Division, Ernest Orlando Lawrence Berkeley National Laboratory. Email: asimmons@lbl.gov. Telephone: 510-486-7106.